



# Central California Ozone Study (CCOS)

## Volume I Conceptual Program Plan

Version 2.1

September 7, 1999

---

# Central California Ozone Study – Volume I

## Conceptual Program Plan

---

Prepared by:

Eric Fujita, Robert Keislar, William Stockwell,  
Hans Moosmuller, David DuBois, Darko Koracin,  
and Barbara Zielinska  
Division of Atmospheric Science  
Desert Research Institute  
2215 Raggio Parkway  
Reno, NV 89512

Saffet Tanrikulu and Andrew Ranzieri  
Planning and Technical Support Division  
California Air Resources Board  
2020 L Street  
Sacramento, CA 95812  
[www.arb.ca.gov](http://www.arb.ca.gov)  
[www.arb.ca.gov/ccaqs/ccos/ccos.htm](http://www.arb.ca.gov/ccaqs/ccos/ccos.htm)

The CCOS Plan was prepared with extensive input from the CCOS Technical Committee, Scientific Advisory Work Group, Meteorological Work Group, and Emission Inventory Coordination Group.

### Technical Committee (Planning Subcommittee)

Andrew Ranzieri, California Air Resources Board  
Saffet Tanrikulu, California Air Resources Board  
Rob DeMandel, Bay Area AQMD  
Bruce Katayama, Sacramento Metropolitan AQMD  
Evan Shipp, San Joaquin Valley Unified APCD  
Phil Roth, Envair  
Jim Sweet, San Joaquin Valley Unified APCD  
Brigette Tollstrup, Sacramento Metropolitan AQMD  
Steve Ziman, Chevron Research and Technology

### Scientific Advisory Work Group

Dan Chang, University of California, Davis  
Dennis Fitz, UCR, CE-CERT  
Robert Harley, University of California, Berkeley  
Mike Kleeman, University of California, Davis  
Gail Tonnesen, University of California, Riverside

### Meteorological Work Group

Saffet Tanrikulu, California Air Resources Board  
Bob Keislar, Desert Research Institute  
David Fairley, Bay Area AQMD  
Tom Umeda, Bay Area AQMD  
Evan Shipp, San Joaquin Valley Unified APCD  
Steve Gouze, California Air Resources Board  
Bruce Katayama, Sacramento Metropolitan AQMD  
Brigette Tollstrup, Sacramento Metropolitan AQMD  
Bob Noon, Monterey Bay Unified AQMD

### Emission Inventory Coordination Group

Linda Murchison, California Air Resources Board  
Dale Shimp, California Air Resources Board  
Cheryl Taylor, California Air Resources Board  
Dennis Wade, California Air Resources Board  
Michael Benjamin, California Air Resources Board  
Phil Martien, Bay Area AQMD  
Toch Mangat, Bay Area AQMD  
Bruce Katayama, Sacramento Metropolitan AQMD  
Brigette Tollstrup, Sacramento Metropolitan AQMD  
Hazel Hoffmann, San Joaquin Valley Unified APCD  
Dave Jones, San Joaquin Valley Unified APCD  
Tom Jordon, San Joaquin Valley Unified APCD  
Scott Nestor, San Joaquin Valley Unified APCD  
Stephen Shaw, San Joaquin Valley Unified APCD  
Gretchen Bennitt, Northern Sierra AQMD  
Dick Johnson, Placer County APCD  
Tom Roemer, San Luis Obispo County APCD  
Larry Green, Yolo-Solano AQMD  
Nancy O'Connor, Yolo-Solano AQMD  
Dave Smith, Yolo-Solano AQMD  
Gordon Garry, Sacramento Area CoG  
Guido Franco, California Energy Commission  
Morris Goldberg, U.S. EPA

## TABLE OF CONTENTS

	<u>Page</u>
List of Tables .....	vi
List of Figures .....	viii
1.0 STUDY OVERVIEW.....	1-1
1.1 Introduction .....	1-1
1.2 CCOS Goals .....	1-3
1.3 CCOS Technical Objectives .....	1-5
1.3.1 Objective A – Planning and Preparation for the CCOS Field Study .....	1-5
1.3.2 Objective B – Emission Inventory Development .....	1-7
1.3.3 Objective C – Preparation, Execution, and Evaluation of Air Quality Simulation Model .....	1-8
1.3.4 Objective D – Data Analysis .....	1-10
1.4 Summary of the Preliminary Conceptual Explanation of Ozone Exceedances in Central and Northern California .....	1-12
1.5 Overview of CCOS Field Measurement Program .....	1-15
1.5.1 Surface Air Quality and Meteorological Monitoring Sites .....	1-16
1.5.2 Surface Meteorological Network .....	1-20
1.5.3 Upper Air Meteorological Network .....	1-21
1.5.4 Aloft Air Quality .....	1-21
1.5.5 Special Studies .....	1-23
1.6 Funding .....	1-24
2.0 BASIS FOR THE FIELD STUDY PLAN .....	2-1
2.1 CCOS Study Area .....	2-1
2.2 Ozone Air Quality Standards and SIP Requirements.....	2-4
2.3 Ambient Trends in Ozone and Precursor Gases .....	2-5
2.3.1 Trends in Ozone Exceedances.....	2-6
2.3.2 Spatial and Temporal Patterns of Ozone Precursors.....	2-7
2.4 Emissions and Source Contributions.....	2-8
2.5 Central California Summer Meteorology and Ozone Climatology.....	2-8
2.5.1 Typical Large-Scale Meteorological Features .....	2-9
2.5.2 Mesoscale Meteorological Features in the CCOS Study Region.....	2-10
2.5.3 Major Transport Couples in Central California .....	2-13
2.5.4 Meteorological Scenarios Associated with Ozone Exceedances .....	2-14
2.6 Atmospheric Transformation and Deposition .....	2-22
2.6.1 Ozone Formation.....	2-22
2.6.2 Heterogeneous Reactions and Ozone - Secondary Aerosol Formation.....	2-33
2.6.3 Role of Ozone Precursors from Natural Sources .....	2-37
2.6.4 Relative Effectiveness of VOC and NO <sub>x</sub> Controls.....	2-37
2.6.5 Atmospheric Deposition.....	2-37
2.7 Conceptual Model of Ozone Episodes and Transport Scenarios of Interest.....	2-38
2.7.1 Current Conceptual Model of Ozone Formation and Transport .....	2-38
2.7.2 Implications of Change in Federal Ozone Standard on Conceptual Model ..	2-39

## TABLE OF CONTENTS (continued)

	<u>Page</u>
2.8 Review of previous SAQM studies and implications for CCOS measurement sites.....	2-38
<b>3.0 REQUIREMENTS FOR AIR QUALITY MODELING SYSTEMS AND DATA ANALYSIS.....</b>	<b>3-1</b>
3.1 Modeling System Inputs.....	3-1
3.1.1 Meteorological Modeling.....	3-1
3.1.2 Emission Inventory Development.....	3-4
3.1.3 Air Quality Modeling.....	3-12
3.2 Model Evaluation.....	3-14
3.2.1 Evaluation of Meteorological Modeling .....	3-14
3.2.2 Evaluation of Emission Inventory Estimates .....	3-15
3.2.3 Air Quality Model Evaluation.....	3-20
3.3 Data Analysis Methods .....	3-21
3.3.1 Accuracy, Precision, Validity, and Equivalence of Field Measurements ....	3-22
3.3.2 Spatial, Temporal, and Statistical Distributions of Air Quality Measurements.....	3-24
3.3.3 Meteorological Transport Phenomena .....	3-26
3.3.4 Meteorological Dispersion Processes .....	3-27
3.3.5 Characterize Pollutant Fluxes.....	3-27
3.3.6 Characterize Chemical and Physical Interactions .....	3-28
3.3.7 Characterize Episodes .....	3-30
3.3.8 Observation-Driven Methods .....	3-31
3.3.9 Contribution of Transported Pollutants to Ozone Violations in Downwind Areas .....	3-31
3.3.10 Contributions of Elevated NO <sub>x</sub> Sources to Downwind O <sub>3</sub> .....	3-32
3.3.11 Deposition Studies.....	3-33
3.3.12 Reformulate the Conceptual Model .....	3-34
<b>4.0 CCOS FIELD MEASUREMENT PROGRAM .....</b>	<b>4-1</b>
4.1 Study Design Principles .....	4-1
4.2 Study Domain.....	4-2
4.3 Study Period.....	4-3
4.4 Supplemental Surface Air Quality and Meteorological Monitoring Sites .....	4-3
4.4.1 Existing Routine Monitoring Network.....	4-4
4.4.2 CCOS Type 1 Supplemental Monitoring Sites .....	4-4
4.4.3 CCOS Type 2 Supplemental Monitoring Sites:.....	4-5
4.4.4 CCOS Research Sites .....	4-6
4.5 Surface Meteorological Network .....	4-7
4.6 Upper Air Meteorological Network .....	4-8
4.7 In-Situ Aircraft Measurements .....	4-9
4.8 Consideration of Alternative Vertical Ozone Measurements.....	4-11
4.9 Measurements for Special Studies .....	4-12

## TABLE OF CONTENTS (continued)

	<u>Page</u>
5.0 BUDGET ESTIMATES .....	5-1
6.0 PROGRAM MANAGEMENT PLAN AND SCHEDULE.....	6-1
6.1 CCOS Management Structure.....	6-1
6.1.1 Policy Committee.....	6-1
6.1.2 Technical Committee .....	6-1
6.1.3 Principal Investigators.....	6-2
6.1.4 Meteorological Working Group .....	6-3
6.1.5 Emissions InventoryWorking Group.....	6-3
6.1.6 Field Coordinator .....	6-3
6.1.7 Quality Assurance Officer.....	6-6
6.1.8 Data Manager .....	6-7
6.1.9 Measurement Investigators .....	6-7
6.1.10 Data Analysis and Modeling Investigators .....	6-8
6.2 Schedule.....	6-9
7.0 REFERENCES .....	7-1
A. MEASUREMENT METHODS	
A.1 Surface Meteorology.....	A-1
A.1.1 Surface Wind Speed and Direction .....	A-1
A.1.2 Surface Relative Humidity .....	A-2
A.1.3 Surface Temperature .....	A-3
A.1.4 Surface Pressure .....	A-3
A.1.5 Solar Radiation.....	A-3
A.2 Upper-Air Wind Speed, Wind Direction, and Temperature .....	A-3
A.2.1 Radar Wind Profilers .....	A-3
A.2.2 Radio-Acoustic Sounding Systems (RASS).....	A-4
A.2.3 Acoustic Sounders (Sodars).....	A-4
A.2.4 Radiosondes .....	A-5
A.2.5 Tethered Balloons .....	A-5
A.2.6 Sonic Anemometers .....	A-6
A.3 Routine Surface Air Quality.....	A-6
A.3.1 Ozone.....	A-7
A.3.2 Nitrogen Oxides .....	A-8
A.3.3 Photochemical Assessment Monitoring Stations (PAMS) Program.....	A-9
A.4 Supplemental Measurements of Ozone .....	A-10
A.4.1 Ozonesondes.....	A-10
A.4.2 Ozone Aloft — Lidar Measurements .....	A-11
A.5 Supplemental Measurements of Oxidized Nitrogen Species .....	A-16
A.5.1 NO <sub>2</sub> and PAN by Gas Chromatography with Luminol Chemiluminescence Detection .....	A-17

## TABLE OF CONTENTS (continued)

	<u>Page</u>
A.5.2 NO <sub>2</sub> and HNO <sub>3</sub> by Tunable Diode Laser Absorption Spectroscopy.....	A-18
A.5.3 NO <sub>2</sub> , HONO, and NO <sub>3</sub> Radical by Differential Optical Absorption Spectroscopy (DOAS).....	A-18
A.5.4 Automated Particle Nitrate Monitor.....	A-18
A.6 In-Situ Instrumented Aircrafts.....	A-20
A.7 Supplemental Measurements of Volatile Organic Compounds .....	A-21
A.7.1 Collection and Analysis of Hydrocarbons and Oxygenated Species .....	A-21
A.7.2 Carbonyl Compounds.....	A-23
A.7.3 C8-C20 Hydrocarbons by Tenax Sampling and Analysis by GC/FID or GC/MS.....	A-24
A.7.4 Continuous Formaldehyde by Fluorescent Detection of Dihydrolutidine Derivative.....	A-24
A.7.5 Continuos GC/MS System.....	A-25
A1 MASTER VOC PARAMETER LIST.....	A1-1
B. QUALITY ASSURANCE.....	B-1
B.1 Quality Assurance Overview .....	B-3
B.2 Data Quality Objectives .....	B-3
B.3 Systems Audits .....	B-4
B.3.1 Field Systems Audits for Surface Monitoring Sites.....	B-4
B.3.2 Field Systems Audits for Aircraft Platforms .....	B-5
B.3.3 Laboratory Systems Audits .....	B-5
B.4 Performance Audits .....	B-5
B.4.1 Field Performance Audits of Surface Monitors .....	B-5
B.4.2 Field Performance Audits for Surface Meteorological Measurements .....	B-6
B.4.3 Field Performance Audits for Upper-Air Meteorology.....	B-7
B.4.4 Field Performance Audits for Aircraft Platforms .....	B-7
B.4.5 Laboratory Performance Audits for Chemical Analysis .....	B-7
C. DATA MANAGEMENT .....	C-1
C.1 Data Specifications .....	C-1
C.2 Data Formats .....	C-2
C.3 File Names.....	C-3
C.4 Validation Flags .....	C-3
C.5 Data Validation Levels.....	C-3
C.6 Internet Server .....	C-5
C.7 Directory Structure .....	C-5
C.8 Data Processing .....	C-6

## LIST OF TABLES

<u>Table No.</u>		<u>Page No.</u>
Table 1.5-1	Supplemental Surface Air Quality and Meteorological Measurements .....	1-25
Table 1.5-2	CCOS Upper-Air Meteorological Measurements .....	1-26
Table 2.1-1	Populations and Areas for Central California Metropolitan Statistical Areas...	2-43
Table 2.3-1a	Linked Master Ozone Monitoring Site List.....	2-44
Table 2.3-1b	Ozone Monitoring Sites Linked in Time for Longer Period of Record.....	2-48
Table 2.3-2	Summary of Trends in Daily 1hr and 8hr Ozone Maxima during May-October, 1990-98 .....	2-49
Table 2.3-3	Annual Maximum of Daily Maximum Ozone Concentrations in Central California During May to October, 1990-98 .....	2-51
Table 2.3-4	Annual Exceedances of the 1-hr and 8-hr Ozone Standards in Central California During May to October, 1990-98 .....	2-56
Table 2.3-5	Average Annual Exceedances of the 1-hr and 8-hr Ozone Standards in Central California by Month May to October, 1990-98 .....	2-61
Table 2.3-6	Average Annual Exceedances of the 1-hr and 8-hr Ozone Standards in Central California by Day-of-the-Week.....	2-66
Table 2.4-1	1996 Daily Average ROG Emissions by Air Basins in the CCOS Domain.....	2-71
Table 2.4-2	1996 Daily Average NOx Emissions by Air Basins in the CCOS Domain.....	2-73
Table 2.5-1	May-October Climate Summaries for Selected Central California Cities (1961-1990 means) .....	2-75
Table 2.5-2	Meteorological Scenarios by Weather Map Inspection .....	2-76
Table 2.5-3	Basin and Subbasin Exceedance Frequencies by Meteorological Scenario .....	2-77
Table 2.5-4	High-Ozone Episodes Identified by the Local Districts for Ozone Seasons 1996-98 .....	2-78
Table 2.5-5	Cluster Analysis Days by Cluster with Subjective Scenario Type .....	2-82
Table 2.5-6	Descriptive Statistics of Meteorological Parameters for Identified Clusters .....	2-84
Table 2.7-1	Number of Exceedances and Ratios of 8-Hour and 1-Hour Parameters.....	2-85
Table 3.1-1	Emission Inventory Roles and Responsibilities.....	3-37
Table 3.1-2	Required Meteorological Files.....	3-38
Table 3.1-3	Typical Chemical Species in an Emission Inventory for Modeling.....	3-38
Table 4.4-1	Supplemental Surface Air Quality and Meteorological Measurements .....	4-15
Table 4.6-1	Upper Air Meteorological Measurements for CCOS.....	4-16
Table 5-1	Summary of Cost Estimates for the CCOS Field Measurement Program.....	5-2

## LIST OF TABLES (continued)

<u>Table No.</u>		<u>Page No.</u>
Table 6.2-1	CCOS Schedule of Milestones.....	6-10
Table A.1-1	Meteorological Sensor Specifications .....	A-26
Table A.1-2	Air Quality Monitoring Site in Northern and Central California .....	A-27
Table A.1-3	PAMS Sites in the CCOS Area .....	A-32
Table A.1-4	PAMS Target Species .....	A-33
Table A.6.1	UCD Instrumentation .....	A-34
Table A.6.2	STI Instrumentation .....	A-35

## LIST OF FIGURES

<u>Figure No.</u>		<u>Page No.</u>
Figure 1.4-1	Mean basin maximum 1-hr ozone for each cluster grouped by cluster and grouped by air basin .....	1-27
Figure 1.4-2	Maximum 1-hr ozone for 126 monitoring stations on 8/12/98, a cluster 1 day.	1-28
Figure 1.4-3	Maximum 8-hr ozone for 126 monitoring stations on 8/12/98, a cluster 1 day.	1-29
Figure 1.4-4	Maximum 1-hr ozone for 126 monitoring stations on 8/12/98, a cluster 2 day.	1-30
Figure 1.4-5	Maximum 8-hr ozone for 126 monitoring stations on 8/12/98, a cluster 2 day.	1-31
Figure 1.4-6	Maximum 1-hr ozone for 126 monitoring stations on 8/12/98, a cluster 3 day.	1-32
Figure 1.4-7	Maximum 8-hr ozone for 126 monitoring stations on 8/12/98, a cluster 3 day.	1-33
Figure 2.1-1	Overall study domain with major landmarks, mountains and passes.....	2-86
Figure 2.1-2	Major political boundaries and air basins within central California.....	2-87
Figure 2.1-3	Major population centers within central California.....	2-88
Figure 2.1-4	Land use within central California from the U.S. Geological Survey.....	2-89
Figure 2.1-5	Major highway routes in central California.....	2-90
Figure 2.3-1	Annual basin maximum of 8-hour daily maximum ozone trends by location type.....	2- 91
Figure 2.3-2	Average 8-hour daily maximum ozone trends in central California by location type .....	2-92
Figure 2.3-3	Weekend/weekday effect on average 1-hour daily maximum ozone in central California by location type .....	2-93
Figure 2.6-1	Overview of ozone production in the troposphere.....	2-94
Figure 2.6-2.	(A) Rate constant for the $O_3 + NO$ reaction with upper and lower bounds. (B) The uncertainty factor, $f(T)$ . ....	2-95
Figure 2.6-3	(A) Rate constant for the $CH_3O_2 + HO_2$ reaction with upper and lower bounds. (B) The uncertainty factor, $f(T)$ .....	2-96
Figure 2.6-4	Atmospheric lifetimes of selected organic compounds with respect to a hydroxyl radical concentration of $7.5 \times 10^6$ molecules cm-3.....	2-97
Figure 2.6-5	Uncertainties in rate parameters for HO radical reactions with alkenes.....	2-98
Figure 2.6-6	Relative sensitivity of ozone to reaction rate constants.....	2-99
Figure 2.6-7	Mean values and $1\sigma$ uncertainties of maximum incremental reactivity values for selected hydrocarbons determined from Monte Carlo simulations.....	2-100

## LIST OF FIGURES (continued)

<u>Figure No.</u>		<u>Page No.</u>
Figure 2.8-2	Plot of 1-hr ozone concentrations in central California at midnight after two simulated days .....	2-101
Figure 2.8-2	Plot of 1-hr ozone concentrations in central California at midnight after two simulated days .....	2-102
Figure 2.8-3	Plot of 1-hr ozone concentrations in central California at noon on the third simulated day .....	2-103
Figure 2.8-4	Plot of 1-hr ozone concentrations in the vertical along a north – south cross section through the center of central California .....	2-104
Figure 2.8-5	Plot of 1-hr ozone concentrations in the vertical along a west – east cross section through central California along a line running from the San Francisco Bay Area through Sacramento to the front range .....	2-105
Figure 2.8-6	Plot of formaldehyde concentrations at midnight after two simulated days....	2-106
Figure 2.8-7	Plot of NO concentrations at 1:00 PM on the second simulated day .....	2-107
Figure 3.1-1	File typically required by photochemical air quality model. ....	3-39
Figure 3.2-1	Average source contribution estimates of ambient hydrocarbons at Rider College, NJ during summer, 1995 by time of day. Source: Fujita and Lu, 1998 .....	3-40
Figure 3.2-3	Wind directional dependence of source contributions by time of the day at Rider College, NJ during summer, 1995.....	3-41
Figure 4.4-1	Existing routine O <sub>3</sub> and NO <sub>x</sub> monitoring sites.....	4-21
Figure 4.4-2	CCOS supplemental air quality and meteorological monitoring sites and Photochemical Assessment Monitoring Stations .....	4-22
Figure 4.5-1	Central California surface meteorological networks and measurement locations. ....	4-23
Figure 4.5-2	Surface meteorological observables measured in the combined central California meteorological network.....	4-24
Figure 4.6-1	Upper air meteorological measurements during the summer campaign, including annual average study sites and NEXRAD (WSR-88D) profilers.....	4-25
Figure 4.6-2	Upper air meteorological measurement network indicating operating agency. ....	4-26
Figure A.1-1	Ultraviolet Absorption Spectra of Ozone, Sulfur Dioxide, and Nitrogen Dioxide .....	A-36
Figure A.1-2	Schematic diagram of NOAA's airborne ozone lidar. ....	A-37